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The nearest definite pair for the Hermitian generalized eigenvalue problem

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Abstract

The generalized eigenvalue problem $Ax = \lambda Bx$ has special properties when (A, B) is a Hermitian and definite pair. Given a general Hermitian pair (A, B) it is of interest to find the nearest definite pair having a specified Crawford number $\delta > 0$. We solve the problem in terms of the inner numerical radius associated with the field of values of $A + iB$. We show that once the problem has been solved it is trivial to rotate the perturbed pair $(A + \Delta A, B + \Delta B)$ to a pair (\tilde{A}, \tilde{B}) for which $\lambda_{\min}(\tilde{B})$ achieves its maximum value δ , which is a numerically desirable property when solving the eigenvalue problem by methods that convert to a standard eigenvalue problem by “inverting B”. Numerical examples are given to illustrate the analysis. © 1999 Elsevier Science Inc. All rights reserved.

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1. Definite Hermitian pairs

Pairs of Hermitian matrices A and B of which one is positive definite play an important role in the generalized eigenproblem $Ax = \lambda Bx$. Assuming,

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without loss of generality, that B is positive definite, the problem is equivalent to the standard Hermitian eigenproblem with matrix $H = B^{-1/2}AB^{-1/2}$, where $C^{1/2}$ denotes the Hermitian positive definite square root of the Hermitian positive definite matrix C . Hence all the eigenvalues are real. Moreover, if $H = Q \operatorname{diag}(\lambda_i) Q^*$ is a spectral decomposition then $X^*BX = I$ and $X^*AX = \operatorname{diag}(\lambda_i)$, where $X = B^{-1/2}Q$, that is, A and B are simultaneously diagonalizable.

These desirable properties extend to the wider class of *definite pairs* (A, B) defined by the property that, for $A, B \in \mathbb{C}^{n \times n}$,

$$\gamma(A, B) := \min_{\substack{z \in \mathbb{C}^n \\ \|z\|_2=1}} \sqrt{(z^*Az)^2 + (z^*Bz)^2} > 0. \quad (1.1)$$

The quantity γ , called the Crawford number, was introduced and exploited in [2, 17]. The following important result applies to definite pairs [17], [18, Th. 6.1.18].

Theorem 1.1. *Let (A, B) be a definite Hermitian pair, and for $\theta \in \mathbb{R}$ let*

$$\begin{aligned} A_\theta &= A \cos \theta + B \sin \theta, \\ B_\theta &= -A \sin \theta + B \cos \theta. \end{aligned} \quad (1.2)$$

Then there is a $\theta \in [0, 2\pi)$ such that B_θ is positive definite and

$$\gamma(A, B) = \lambda_{\min}(B_\theta).$$

It is easy to see from the proof of Theorem 1.1 that, in fact, $\gamma(A, B) = \max_\theta \lambda_{\min}(B_\theta)$. If we regard the eigenvalues of a matrix pair (A, B) as pairs (α, β) satisfying $\det(\beta A - \alpha B) = 0$, then the eigenvalues (α, β) of (A, B) and (a_θ, b_θ) of (A_θ, B_θ) are related by

$$\begin{bmatrix} \beta \\ \alpha \end{bmatrix} \begin{bmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{bmatrix} \begin{bmatrix} b_\theta \\ a_\theta \end{bmatrix}. \quad (1.3)$$

It follows from the theorem that definite pairs have real eigenvalues and are simultaneously diagonalizable. The definiteness of (A, B) is equivalent to the field of values of $A + iB$ not containing the origin (see Section 2), which is equivalent to the field of values lying in an open half plane. Moreover, $A_\theta + iB_\theta = e^{-i\theta}(A + iB)$ in (1.2).

Three problems arise in the numerical solution of the Hermitian eigenproblem. First, it is desirable to be able to check numerically whether a given Hermitian pair is definite. Second, because of rounding and measurement errors, it may happen that a Hermitian pair that is expected to be definite fails to

be definite in practice. In this situation it is natural to compute the nearest definite pair and to solve the eigenproblem for the definite pair. This nearest definite pair problem adds to the many existing matrix nearness problems [8] and generalizes the problem of finding the nearest symmetric positive definite matrix [7].

The third problem arises because existing direct methods are able to exploit the Hermitian structure only when one of the matrices is positive definite. Therefore given a definite pair it is desirable to be able to find an angle θ so that $\lambda_{\min}(B_\theta) > 0$ in (1.2), so that numerical methods can be applied to the rotated pair. A standard method for solving the eigenproblem when B is positive definite is to compute the Cholesky factorization $B = R^*R$ and to reduce the problem to the eigenproblem for the Hermitian matrix $C = R^{-*}AR^{-1}$ [15] (Section 15.4). Error analysis for the formation of C implies that the computed eigenvalues are then at best the exact ones of $C + \Delta C$ with $\|\Delta C\|_2 \leq u\|A\|_2\lambda_{\min}(B)^{-1}$, where u is the unit roundoff. Hence a reasonable strategy to maximize the accuracy of the computed eigenvalues is to choose θ to minimize $\|A_\theta\|\lambda_{\min}(B_\theta)^{-1}$; more simply, we can maximize $\lambda_{\min}(B_\theta)$, to yield the maximal value $\gamma(A, B)$. The same maximization problem is also relevant to the computation of error bounds [10]. (The problem of minimizing $\lambda_{\max}(B_\theta)/\lambda_{\min}(B_\theta)$ is also relevant in the perturbation theory; see [14].)

In this work we solve these three problems. In Section 3 we obtain formulae for the nearest definite pair with a given Crawford number and the corresponding distance. The result is expressed in terms of the inner numerical radius associated with the field of values. In Section 2 we present the necessary background on the field of values and obtain a formula for the inner numerical radius. As a by-product of computation of the nearest definite pair we obtain immediately an angle θ in Theorem 1.1 such that $\lambda_{\min}(B_\theta)$ achieves the maximal value $\gamma(A, B)$. In Section 4 we give the overall algorithm and some numerical examples.

2. Field of values

The *field of values* (or numerical range) of a general matrix $A \in \mathbb{C}^{n \times n}$ is defined by

$$F(A) = \left\{ \frac{z^*Az}{z^*z} : 0 \neq z \in \mathbb{C}^n \right\}.$$

The magnitude of the largest element of $F(A)$ is called the *numerical radius*:

$$r_{\max}(A) = \max\{|w| : w \in F(A)\}.$$

The numerical radius of A can be interpreted as the radius of the smallest circle centred at the origin that contains $F(A)$. The numerical radius is approximated to within a factor 2 by the 2-norm of the matrix [9, p. 331]:

$$\frac{1}{2} \|A\|_2 \leq r_{\max}(A) \leq \|A\|_2. \quad (2.1)$$

Note that the maximum defining the numerical radius is always attained at a point on the boundary of the field of values. Also of interest, though less commonly considered, is the minimum absolute value of a point on the boundary, which we call the *inner numerical radius*:

$$\zeta(A) = \min\{|w| : w \text{ is on the boundary of } F(A)\}.$$

This quantity is not to be confused with

$$r_{\min}(A) = \min\{|w| : w \in F(A)\}.$$

When the origin is not contained in the field of values, $\zeta(A) = r_{\min}(A)$. When the field of values does contain the origin, $r_{\min}(A) = 0$ while $\zeta(A)$ is the radius of the largest circle centred at the origin and contained within $F(A)$. Some authors call $r_{\min}(A)$ the inner numerical radius [13], but because it provides useful radius information when $0 \in F(A)$ we think it is more natural to give this name to $\zeta(A)$.

Note that $\gamma(A, B)$ in (1.1) can be expressed as $\gamma(A, B) = r_{\min}(A + iB)$ and hence can be expressed in terms of $\zeta(A)$.

Some attention has been given to computing the numerical radius. Watson [19] describes a method related to the power method, and He and Watson [6] show how to overcome the problem with this method of convergence to local maxima.

To see how to evaluate $\zeta(A)$, write $A = (A + A^*)/2 + (A - A^*)/2 =: H + S$, where H is Hermitian and S skew-Hermitian. For any z we have

$$z^*Az = \underbrace{z^*Hz}_{\text{real}} + \underbrace{z^*Sz}_{\text{pure imaginary}},$$

which implies that for $w \in F(A)$

$$\lambda_{\min}(H) \leq \operatorname{Re}(w) \leq \lambda_{\max}(H),$$

where λ_{\min} and λ_{\max} denote the smallest and largest eigenvalues, respectively, of a Hermitian matrix. These bounds are attained when w is the Rayleigh quotient $z^*Az/(z^*z)$ with z an eigenvector of H corresponding to $\lambda_{\min}(H)$ or $\lambda_{\max}(H)$; note that this point lies on the boundary of $F(A)$. Now consider $A_\theta = e^{-i\theta}A$. The field of values of A_θ is just that of A rotated clockwise through θ radians about the origin, so $\zeta(A_\theta) = \zeta(A)$. Applying the above argument to A_θ we obtain

$$\lambda_{\min}(H_\theta) \leq \operatorname{Re}(e^{-i\theta}w) \leq \lambda_{\max}(H_\theta), \quad w \in F(A), \quad (2.2)$$

where, again, each bound is attained at a point on the boundary of $F(A)$.

Theorem 2.1. *The inner numerical radius satisfies*

$$\zeta(A) = \left| \min_{0 \leq \theta \leq 2\pi} \lambda_{\max}(H_\theta) \right|, \quad (2.3)$$

where $A_\theta = e^{-i\theta}A$ and $H_\theta = (A_\theta + A_\theta^*)/2$. Let the minimum be attained at $\theta = \theta_*$. Then $0 \in F(A)$ if and only if $\lambda_{\max}(H_{\theta_*}) \geq 0$, and the point $\zeta(A)e^{i\phi}$ is on the boundary of $F(A)$ where

$$\phi = \begin{cases} \theta_* & \text{if } 0 \in F(A), \\ \theta_* + \pi & \text{if } 0 \notin F(A). \end{cases}$$

Proof. Consider, first, the case where $0 \in F(A)$. Then $0 \in F(A_\theta)$ for all θ , so $\lambda_{\max}(H_\theta) \geq 0$ for all θ , by (2.2). Since $F(A)$ is convex, every point w on the boundary of $F(A)$ having minimal modulus gives equality in the right-hand side inequality of (2.2) for some θ , and it follows that

$$\zeta(A) \geq \left| \min_{0 \leq \theta \leq 2\pi} \lambda_{\max}(H_\theta) \right|. \quad (2.4)$$

If $\zeta(A)$ is attained at the point $re^{i\phi}$ on the boundary of $F(A)$, then equality is attained in (2.4) for $\theta = \phi$.

If $F(A)$ does not contain the origin then $\lambda_{\max}(H_\theta)$ takes both positive and negative values for $\theta \in [0, 2\pi]$. It is easy to see that if $\zeta(A)$ is attained at the point $re^{i\phi}$ on the boundary of $F(A)$ then (2.3) holds with the minimum being attained when $\theta = \phi - \pi$ and that $\lambda_{\max}(H_\theta)$ is negative. \square

Theorem 2.1 can also be formulated in terms of $\lambda_{\min}(H_\theta)$.

3. The nearest definite pair

Suppose that the Hermitian pair (A, B) is not definite. We wish to find the distance to the nearest definite pair with a given positive value of γ , which we define by

$$d_\delta(A, B) = \min\{\|[\Delta A \ \Delta B]\|_2 : \gamma(A + \Delta A, B + \Delta B) \geq \delta\}, \quad \delta > 0. \quad (3.1)$$

We require only inequality rather than equality in the definition so that $d_\delta(A, B) = 0$ when (A, B) is a definite pair with $\gamma(A, B) > \delta$. The quantity $\|[\Delta A \ \Delta B]\|_2$ is not the only possible measure of the distance between (A, B) and $(A + \Delta A, B + \Delta B)$. A measure based on projectors is attractive for perturbation

theory; see [5, 12], for example. However, our choice is natural in the context of floating point computation, where relative errors in A and B are expected and relative perturbations are easily interpreted. Note that for nonzero A and B ,

$$Ax = \lambda Bx \iff \left(\frac{A}{\|A\|_2}\right)x = \left(\lambda \frac{\|B\|_2}{\|A\|_2}\right)\left(\frac{B}{\|B\|_2}\right)x.$$

Hence we can assume that $\|A\|_2 = \|B\|_2 = 1$ without loss of generality, so that $\|[\Delta A \ \Delta B]\|_2$ is a measure of the *relative* change in A and B .

The problem (3.1) has an elegant solution in terms of the inner numerical radius.

Theorem 3.1. *Let $A, B \in \mathbb{C}^{n \times n}$ be Hermitian and let $C = A + iB$ and $A_\phi = A \cos \phi + B \sin \phi$. Let $\min_{0 \leq \phi \leq 2\pi} \lambda_{\max}(A_\phi)$ be attained at the angle θ and let A_θ have the spectral decomposition*

$$A_\theta = Q \operatorname{diag}(\mu_i) Q^*, \quad \mu_n \leq \mu_{n-1} \leq \dots \leq \mu_1.$$

If $0 \in F(C)$ (or, equivalently, $\mu_1 \geq 0$) then

$$d_\delta(A, B) = \delta + \mu_1 = \delta + \zeta(C).$$

If $0 \notin F(C)$ (or, equivalently, $\mu_1 < 0$) then

$$d_\delta(A, B) = \max(\delta + \mu_1, 0) = \max(\delta - \zeta(C), 0).$$

In both cases, two sets of optimal perturbations in (3.1) are

$$\begin{aligned} \Delta A_1 &= \cos \theta Q \operatorname{diag}(\min(-\delta - \mu_i, 0)) Q^*, \\ \Delta B_1 &= \sin \theta Q \operatorname{diag}(\min(-\delta - \mu_i, 0)) Q^* \end{aligned} \tag{3.2}$$

and

$$\Delta A_2 = -d_\delta(A, B) \cos \theta I, \quad \Delta B_2 = -d_\delta(A, B) \sin \theta I. \tag{3.3}$$

Proof. First, we consider the case $0 \in F(C)$. Write $\Delta C = \Delta A + i\Delta B$. Definition (1.1) of $\gamma(A, B)$ shows that our task is to find Hermitian perturbations ΔA and ΔB such that $r_{\min}(C + \Delta C) = \delta$ and $\|[\Delta A \ \Delta B]\|_2$ is minimized. If ΔC is an optimal perturbation then every point in the convex set $F(C + \Delta C)$ has modulus at least δ , with equality for at least one point, so there is a line p whose minimal distance to the origin is δ such that $F(C + \Delta C)$ lies entirely in the closed half plane H defined by p that excludes the origin. Let the line perpendicular to p passing through the origin intersect the boundary of $F(C)$ in the complement of H at $w = z^* C z$ ($z^* z = 1$); if there are two such points, take the one furthest from p . Then when C is perturbed to $C + \Delta C$ this point must move distance at least $|w| + \delta$; see Fig. 1. Hence

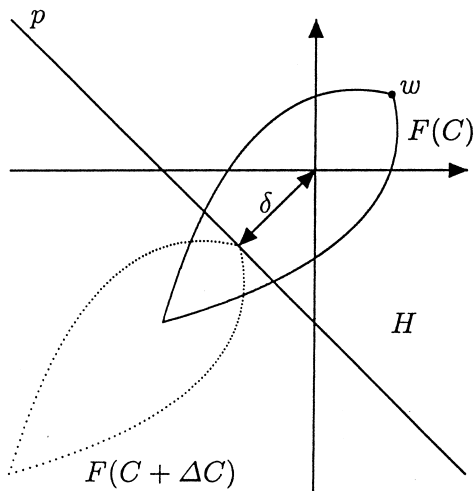


Fig. 1. Diagram for first part of proof of Theorem 3.1.

$$|z^* \Delta C z| = |z^*(C + \Delta C)z - z^* C z| \geq |w| + \delta \geq \zeta(C) + \delta.$$

Now, using a trick from [11],

$$\begin{aligned} |z^* \Delta C z| &= |z^* \Delta A z + i z^* \Delta B z| \\ &= ((z^* \Delta A z)^2 + (z^* \Delta B z)^2)^{1/2} \\ &= \max_{\theta} [z^* \Delta A z \ z^* \Delta B z] \begin{bmatrix} \cos \theta \\ \sin \theta \end{bmatrix} \\ &= \max_{\theta} z^* [\Delta A \ \Delta B] \begin{bmatrix} \cos \theta I \\ \sin \theta I \end{bmatrix} z \\ &\leq \max_{\theta} \left\| [\Delta A \ \Delta B] \begin{bmatrix} \cos \theta I \\ \sin \theta I \end{bmatrix} \right\|_2 \\ &\leq \|[\Delta A \ \Delta B]\|_2. \end{aligned}$$

Hence

$$\|[\Delta A \ \Delta B]\|_2 \geq \zeta(C) + \delta. \quad (3.4)$$

With θ as specified in the statement of the theorem define $A_{\theta} + iB_{\theta} = e^{-i\theta}(A + iB)$, so that $A_{\theta} = A \cos \theta + B \sin \theta$ and $\zeta(A_{\theta} + iB_{\theta}) = \zeta(A + iB)$. Note that $F(A_{\theta} + iB_{\theta})$ is $F(A + iB)$ rotated θ radians clockwise about the origin. Applying Theorem 2.1 to C and recalling that $0 \in F(C)$, we find that $\zeta(A_{\theta} + iB_{\theta})$ is attained at the point in the complex plane

$$(\mu_1, 0) = (q_1^* A_\theta q_1, q_1^* B_\theta q_1),$$

where $\mu_1 \geq 0$ and q_1 is the first column of Q . Let

$$\Delta A_\theta = Q \operatorname{diag}(\min(-\delta - \mu_1, 0)) Q^*, \quad \Delta B_\theta = 0.$$

Then all the eigenvalues of $A_\theta + \Delta A_\theta$ are less than or equal to $-\delta$ and

$$(q_1^* (A_\theta + \Delta A_\theta) q_1, q_1^* (B_\theta + \Delta B_\theta) q_1) = (-\delta, 0),$$

so it follows that

$$\gamma(A_\theta + \Delta A_\theta, B_\theta + \Delta B_\theta) = \delta.$$

Now define ΔA and ΔB by

$$A + \Delta A + i(B + \Delta B) = e^{i\theta}(A_\theta + \Delta A_\theta + i(B_\theta + \Delta B_\theta)).$$

Then

$$\gamma(A + \Delta A, B + \Delta B) = \gamma(A_\theta + \Delta A_\theta, B_\theta + \Delta B_\theta) = \delta.$$

Moreover,

$$[\Delta A \ \Delta B] = [\Delta A_\theta \ \Delta B_\theta] \begin{bmatrix} \cos \theta I & \sin \theta I \\ -\sin \theta I & \cos \theta I \end{bmatrix}$$

and, since the third matrix in this equation is orthogonal, it follows that

$$\|[\Delta A \ \Delta B]\|_2 = \|[\Delta A_\theta \ \Delta B_\theta]\|_2 = \delta + \mu_1 = \delta + \zeta(C).$$

Thus ΔA and ΔB are feasible perturbations that attain the lower bound in (3.4), and so are optimal. The perturbations (3.3) correspond to

$$\Delta A_\theta = Q \operatorname{diag}(-\delta - \mu_1) Q^* = -(\delta + \zeta(C))I, \quad \Delta B_\theta = 0,$$

and are easily seen to provide another solution.

Now suppose that $0 \notin F(C)$. Note that only in this case can (A, B) already be a definite pair and hence $d_\delta(A, B)$ be zero. If $\zeta(C) \geq \delta$ then, trivially, $d_\delta(C) = 0$ and the distance and perturbations in the statement of the theorem are, correctly, all zero. Therefore we can assume that $\zeta(C) < \delta$. Define $A_\theta + iB_\theta$ as in the first part. Note that, by Theorem 2.1, $F(A_\theta + iB_\theta)$ lies in the open left half plane and $w = -\zeta(A_\theta + iB_\theta)$ is on the boundary of $F(A_\theta + iB_\theta)$. The perturbations ΔC must move w to the boundary or exterior of the circle centre 0 and radius δ , therefore w must move a distance at least $\delta + \mu_1$. As in the first part, this leads to the bound $\|[\Delta A \ \Delta B]\|_2 \geq \delta + \mu_1$, and the rest of the proof is very similar to that of the first part. \square

4. Numerical algorithm and experiments

The following algorithm solves the problems described in Section 1: it finds the nearest definite pair with a given Crawford number δ and then rotates that definite pair to maximize the smallest eigenvalue of the B matrix. The latter computation is trivial once we know the location of a point at which the inner numerical radius is attained for the perturbed pair.

Algorithm 1. Given Hermitian matrices $A, B \in \mathbb{C}^{n \times n}$ and a parameter $\delta > 0$ this algorithm computes the distance $d_\delta(A, B)$ in (3.1) and corresponding optimal perturbations ΔA and ΔB , together with an angle θ such that (\tilde{A}, \tilde{B}) is a definite pair with $\lambda_{\min}(\tilde{B}) = \delta$, where $\tilde{A} + i\tilde{B} = e^{-i\theta}(A + \Delta A, B + \Delta B)$.

1. Find the global minimizing point ψ of $\lambda_{\max}(A \cos \phi + B \sin \phi)$. Compute the spectral decomposition $A_\psi = Q \text{diag}(\mu_i) Q^*$, where $\mu_n \leq \mu_{n-1} \leq \dots \leq \mu_1$.
2. $\Delta A = \cos \psi Q \text{diag}(\min(-\delta - \mu_i, 0)) Q^*$, $\Delta B = \sin \psi Q \text{diag}(\min(-\delta - \mu_i, 0)) Q^*$, $d_\delta(A, B) = \max(\delta + \mu_1, 0)$.
3. $\theta = \pi/2 - \psi$.

The main question in implementing Algorithm 1 is how to compute ψ . The function $f(\phi) = \lambda_{\max}(A \cos \phi + B \sin \phi)$ can have many local minima on $[0, 2\pi]$. Fig. 2 plots f over $[0, 2\pi]$ for a random A and B of order 8. Local minima can be

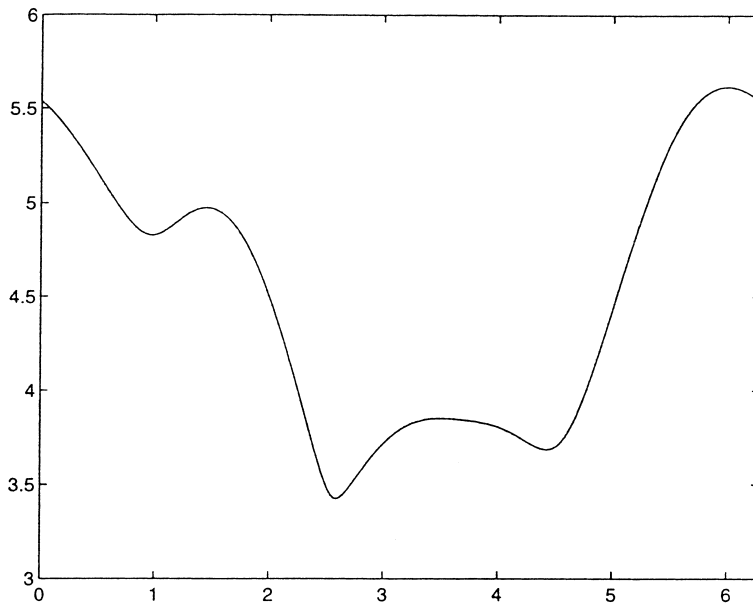


Fig. 2. $f(\phi) = \lambda_{\max}(A \cos \phi + B \sin \phi)$ for a random Hermitian A and B .

found using standard numerical methods [16, Ch. 10]. However, we require the global minimum, which none of the standard methods guarantees to find. We have therefore taken a simple, though expensive approach: we find the minimum on a grid of p equally spaced points by setting

$$\psi = \operatorname{argmin}\{\lambda_{\max}(A \cos \phi + B \sin \phi) : \phi = 2\pi j/p, j = 0 : p-1\}. \quad (4.1)$$

We present three numerical examples to illustrate Algorithm 1. In each case we took $p = 100$ in (4.1). By convention, when we refer to the field of values of (A, B) we mean that of $A + iB$. All the computations were done in MATLAB 5.2, which has unit roundoff $u \approx 1.1 \times 10^{-16}$. In Algorithm 1 eigensystems were computed using the QR algorithm.

In the first example, adapted from [18, p. 281],

$$A = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad B = \begin{bmatrix} 0 & 2 \\ 2 & 0 \end{bmatrix}. \quad (4.2)$$

The pair (A, B) is not definite and has eigenvalues $\pm i/2$. The boundary of the field of values of (A, B) is easily seen to be the ellipse $4(\operatorname{Re} z)^2 + (\operatorname{Im} z)^2 = 4$, and hence $\zeta(A + iB) = 1$ and $d_\delta(A, B) = 1 + \delta$. We applied Algorithm 1 with $\delta = 0.25$ and obtained $d_\delta(A, B) = 1.25$ exactly. Fig. 3 plots the field of values for the original pair (A, B) , that for the two perturbed pairs $(A + \Delta A_1, B + \Delta B_1)$ and $(A + \Delta A_2, B + \Delta B_2)$ in (3.2) and (3.3) and finally that for the rotated pair (\tilde{A}, \tilde{B}) (based on $(A + \Delta A_1, B + \Delta B_1)$) for which $\lambda_{\min}(\tilde{B})$ attains the maximal value $\gamma(A + \Delta A_1, B + \Delta B_1)$. For each plot, points at which the inner numerical radius and the numerical radius are attained are marked by a diamond and a square, respectively, and the eigenvalues of “ $A + iB$ ” (not those of “ (A, B) ”) are marked by crosses.

The second example has $n = 7$ with $A = \operatorname{diag}(-3 : 3)$ and B the Cauchy matrix $b_{ij} = 1/(i + j)$, except that we modified $b_{11} = b_{nn} = -1$ in order to make the pair indefinite. With $\delta = 10^{-8}$ we found that $d_\delta(A, B) = 0.812$. The plots are shown in Fig. 4. The smallest eigenvalues of B is -1.17 , so if we try to restore definiteness of the pair by perturbing B to make it positive definite then we must make a perturbation of 2-norm at least $1.17 > d_\delta(A, B)$ [7].

The third example illustrates the numerical benefits to be gained by rotating a pair in which B is already positive definite in order to maximize $\lambda_{\min}(B_\theta)$. Here, with $n = 10$,

$$\begin{aligned} A &= (|i - j|) && \text{(Fiedler matrix),} \\ B &= U^T U, && U \text{ unit upper triangular with } u_{ij} = -1, j > i \\ &&& \text{(Moler matrix).} \end{aligned} \quad (4.3)$$

The pair (A, B) is definite with $\gamma(A, B) = 0.18$ and $\lambda_{\min}(B) = 8.6 \times 10^{-6}$. We solved the eigenproblem for (A, B) using the Cholesky factorization method described in Section 1. Then we used Algorithm 1 (omitting step 2) to find the

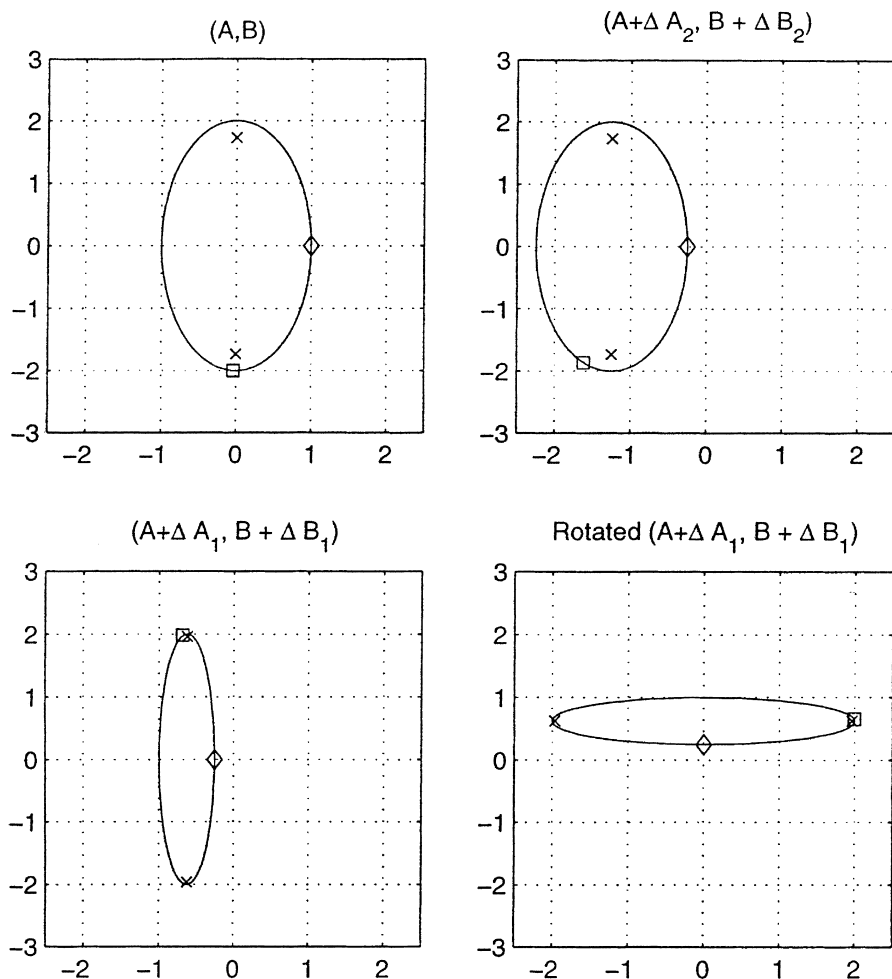


Fig. 3. Fields of values for problem (4.2); $\delta = 0.25$. Inner numerical radius attained at '◇' and numerical radius attained at '□'.

angle θ such that $\lambda_{\min}(B_\theta) = \gamma(A, B)$; we solved the eigenproblem for (A_θ, B_θ) using the Cholesky factorization method and transformed the eigenvalues μ_i back to those for (A, B) using the formula $\lambda_i = \tan(\tan^{-1}(\mu_i) - \theta)$. Table 1 gives the relative errors in the two sets of computed eigenvalues. For the Cholesky method on (A, B) the computed eigenvalues have relative errors ranging between three and five orders of magnitude larger than the unit roundoff u , corresponding to $\lambda_{\min}(B)^{-1}$ being of order 10^5 . However, the Cholesky method applied to (A_θ, B_θ) , for which $\lambda_{\min}(B_\theta) = \gamma(A, B) = 0.18$ yields much more

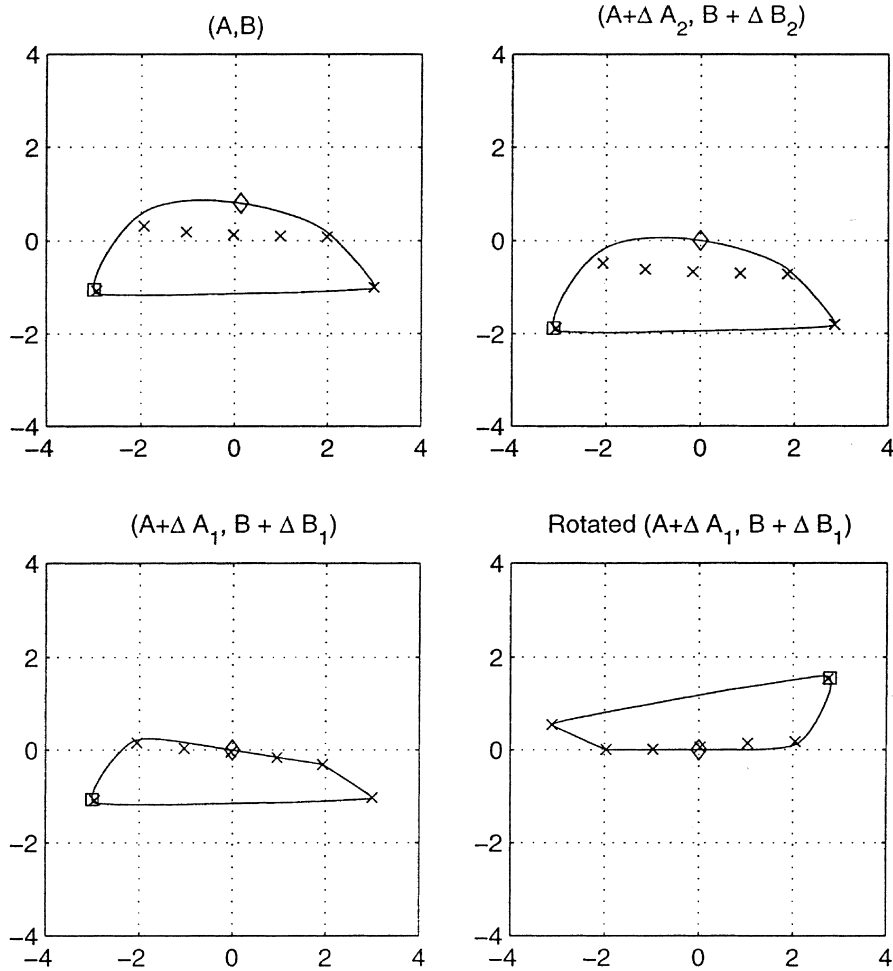


Fig. 4. Fields of values for second example; $\delta = 10^{-8}$. Inner numerical radius attained at '◇' and numerical radius attained at '□'.

accurate eigenvalues: only the largest eigenvalues has more than one incorrect significant figure, and this loss of accuracy is caused by ill condition of the tan transformation (the transformation (1.3) also suffers from this ill condition). We also tried using complete pivoting in the Cholesky factorization method applied to (A, B) , obtaining the relative errors listed in the final column of Table 1. Complete pivoting tends to make the reduced eigenproblem graded, and the QR algorithm often yields higher accuracy for graded matrices [15]. In our example, the accuracy is significantly improved, though not quite as much as for the rotation technique.

Table 1
Relative errors in computed eigenvalues from the Cholesky method for (4.2)

λ_i	(A, B)	(A_θ, B_θ)	(A, B) with pivoting
$-5.4\text{e} + 0$	$8.5\text{e} - 13$	$3.3\text{e} - 15$	$3.4\text{e} - 14$
$-1.2\text{e} + 0$	$2.9\text{e} - 12$	$1.7\text{e} - 15$	$2.3\text{e} - 14$
$-7.6\text{e} - 1$	$8.4\text{e} - 12$	$4.4\text{e} - 16$	$3.1\text{e} - 14$
$-5.4\text{e} - 1$	$1.8\text{e} - 11$	$4.1\text{e} - 15$	$1.4\text{e} - 14$
$-4.0\text{e} - 1$	$3.2\text{e} - 11$	$2.5\text{e} - 15$	$9.0\text{e} - 15$
$-3.2\text{e} - 1$	$3.8\text{e} - 11$	$1.7\text{e} - 15$	$5.2\text{e} - 16$
$-2.7\text{e} - 1$	$4.5\text{e} - 11$	$8.2\text{e} - 16$	$1.8\text{e} - 15$
$-2.4\text{e} - 1$	$3.1\text{e} - 11$	$4.5\text{e} - 15$	$3.9\text{e} - 14$
$-2.3\text{e} - 1$	$1.1\text{e} - 11$	$6.1\text{e} - 16$	$1.8\text{e} - 14$
$4.6\text{e} + 5$	$2.9\text{e} - 11$	$1.8\text{e} - 10$	$1.9\text{e} - 11$

In related work, Crawford and Moon [3,4] present a bisection-like algorithm for computing θ such that B_θ is positive definite, for a definite pair (A, B) . The main computational cost of their algorithm is a Cholesky factorization in each step to test the definiteness of B_θ for the current estimate of θ . They do not attempt to maximize $\lambda_{\min}(B_\theta)$ and their algorithm can take $O(n)$ steps and therefore can require $O(n^4)$ flops.

We have left two important computational issues unexplored, namely, how to reliably and efficiently find the global minimizing point of $f(\phi) = \lambda_{\max}(A \cos \phi + B \sin \phi)$ and how to evaluate this function efficiently (for example, when A and B are large and sparse). One possibility is to apply a local minimization method starting from the best point found from the grid search (4.5). These issues arise also in other problems (see, for example, [1] for the evaluation of λ_{\max}) and it is desirable to exploit the particular structure of our problem in addressing them.

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References

- [1] T. Braconnier, N.J. Higham, Computing the field of values and pseudospectra using the Lanczos method with continuation, *BIT* 36 (3) (1996) 422–440.
- [2] C.R. Crawford, A stable generalized eigenvalue problem, *SIAM J. Numer. Anal.* 13 (6) (1976) 854–860.
- [3] C.R. Crawford, ALGORITHM 646 PDFIND: A routine to find a positive definite linear combination of two real symmetric matrices, *ACM Trans. Math. Software* 12 (1986) 278–282.

- [4] C.R. Crawford, Y.S. Moon, Finding a positive definite linear combination of two Hermitian matrices, *Linear Algebra Appl.* 51 (1983) 37–48.
- [5] L. Elsner, Ji guang Sun, Perturbation theorems for the generalized eigenvalue problem, *Linear Algebra Appl.* 48 (1982) 341–357.
- [6] Chunyang He, G.A. Watson, An algorithm for computing the numerical radius, *IMA J. Numer. Anal.* 17 (1997) 329–342.
- [7] N.J. Higham, Computing a nearest symmetric positive semidefinite matrix, *Linear Algebra Appl.* 103 (1988) 103–118.
- [8] N.J. Higham, Matrix nearness problems and applications, in: M.J.C. Gover, S. Barnett (Eds.), *Applications of Matrix Theory*, Oxford University Press, Oxford, 1989, pp. 1–27.
- [9] R.A. Horn, C.R. Johnson, *Matrix Analysis*, Cambridge University Press, Cambridge, 1985. xiii+561 pp. ISBN 0-521-30586-1.
- [10] Chi-Kwong Li, R. Mathias, Generalized eigenvalues of a definite Hermitian matrix pair, *Linear Algebra and Appl.* 271 (1998) 309–321.
- [11] Ren-Cang Li, A perturbation bound for definite pencils, *Linear Algebra and Appl.* 179 (1993) 191–202.
- [12] Ren-Cang Li, On perturbations of matrix pencils with real spectra, *Math. Comp.* 62 (205) (1994) 231–265.
- [13] J. Maroulas, P. Psarrakos, The boundary of the numerical range of matrix polynomials, *Linear Algebra and Appl.* 267 (1997) 101–111.
- [14] B.N. Parlett, Symmetric matrix pencils, *J. Comp. Appl. Math.* 38 (1991) 373–385.
- [15] B.N. Parlett, *The Symmetric Eigenvalue Problem*, Society for Industrial and Applied Mathematics, Philadelphia, PA, USA, 1998, pp. xxiv+398 (unabridged, amended version of book first published by Prentice-Hall in 1980, ISBN 0-89871-402-8).
- [16] W.H. Press, S.A. Teukolsky, W.T. Vetterling, B.P. Flannery, *Numerical Recipes in FORTRAN: The Art of Scientific Computing*, 2nd ed., Cambridge University Press, Cambridge, 1992, pp. xxvi+963, ISBN 0 521 43064 X.
- [17] G.W. Stewart, Perturbation bounds for the definite generalized eigenvalue problem, *Linear Algebra and Appl.* 23 (1979) 69–85.
- [18] G.W. Stewart, Ji-guang Sun, *Matrix Perturbation Theory*, Academic Press, London, 1990, pp. xv+365, ISBN 0-12-670230-6.
- [19] G.A. Watson, Computing the numerical radius, *Linear Algebra and Appl.* 234 (1996) 163–172.